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Publication date:
1997

Document Version
Publisher's PDF, also known as Version of record

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September 1999 (rev. May 2002)

Computer representation of differential quotients

Many engineering problems can be characterized as the solution to a partial differential equation (PDE). However, in many cases such solutions cannot be found analytically - especially if the boundary conditions of the problems are not simple/regular. This is the main reason for adopting numerical techniques to find solutions.

Due to the finite size of memory on a computer, it is not possible to represent the differential derivatives of the PDE in an exact form. The reason is that differential quotients are defined over infinitely short intervals. The computer representation is incremental in its nature, and thus, a so-called discretization needs to be introduced. This means, that for example derivatives at points are approximated by difference quotients over small intervals. The notion of *finite differences* is introduced.

A common example of a PDE, which is very useful in this course, is the transient heat conduction equation - a parabolic PDE:

$$\frac{\partial T}{\partial t} = a \frac{\partial^2 T}{\partial x^2} \qquad (1)$$

where T is the temperature, K
t is time, s
x is the one-dimensional space coordinate, m
a is the thermal diffusivity, m^2/s

Here we need to find difference approximations of the first order derivative of temperature with respect to time, t, and of the second order derivative of temperature with respect to the one-dimensional space coordinate, x.

Taylor expansion

Assume, the temperature T depends on the variable u (for which we will later insert either time t or space coordinate x): $T(u)$.

Taylor expansion gives the temperature at u+Δu:

$$T(u+\Delta u)=$$
$$T(u)+\frac{\Delta u}{1!}T'(u)+\frac{(\Delta u)^2}{2!}T''(u)+\frac{(\Delta u)^3}{3!}T'''(u)+\frac{(\Delta u)^4}{4!}T''''(u)+... \qquad (2)$$

And similarly for the temperature at u-Δu:

$$T(u-\Delta u)=$$
$$T(u)-\frac{\Delta u}{1!}T'(u)+\frac{(\Delta u)^2}{2!}T''(u)-\frac{(\Delta u)^3}{3!}T'''(u)+\frac{(\Delta u)^4}{4!}T''''(u)-... \qquad (3)$$

The first order partial derivative of T with respect to u can be isolated directly from Equation 2:

$$T'(u)=\frac{\partial T}{\partial u}=\frac{\mathrm{T\,(u+\Delta u)\ -\ T\,(u)}}{\Delta \mathrm{u}}\ +\ \mathrm{O}\,(\Delta \mathrm{u}) \qquad (4)$$

Or it can be isolated directly from Equation 3 as:

$$T'(u)=\frac{\partial T}{\partial u}=\frac{\mathrm{T\,(u)\ -\ T\,(u-\Delta u)}}{\Delta \mathrm{u}}\ +\ \mathrm{O}\,(\Delta \mathrm{u}) \qquad (5)$$

If Equation 3 is subtracted from Equation 2, the following Equation results:

$$T\,(u+\Delta u)\ -\ T\,(u-\Delta u)=2\,\frac{\Delta u}{1!}\,T'(u)\ +\ 2\,\frac{(\Delta u\,)^3}{3!}\,T'''(u)\ +\ ... \qquad (6)$$

Isolating the partial derivative of T with respect to u from Equation 6 yields:

$$T'(u)=\frac{\partial T}{\partial u}=\frac{\mathrm{T\,(u+\Delta u)\ -\ T\,(u-\Delta u)}}{2\,\Delta \mathrm{u}}\ +\ \mathrm{O}\,[(\Delta \mathrm{u}\,)^2] \qquad (7)$$

The approximations of the first order derivative presented as the first terms on the right hand sides of Equations 4, 5, and 7 (marked in bold), are known as the *forward*, *backward* and *central* forms, respectively. The three approximations are illustrated in Figure 1.

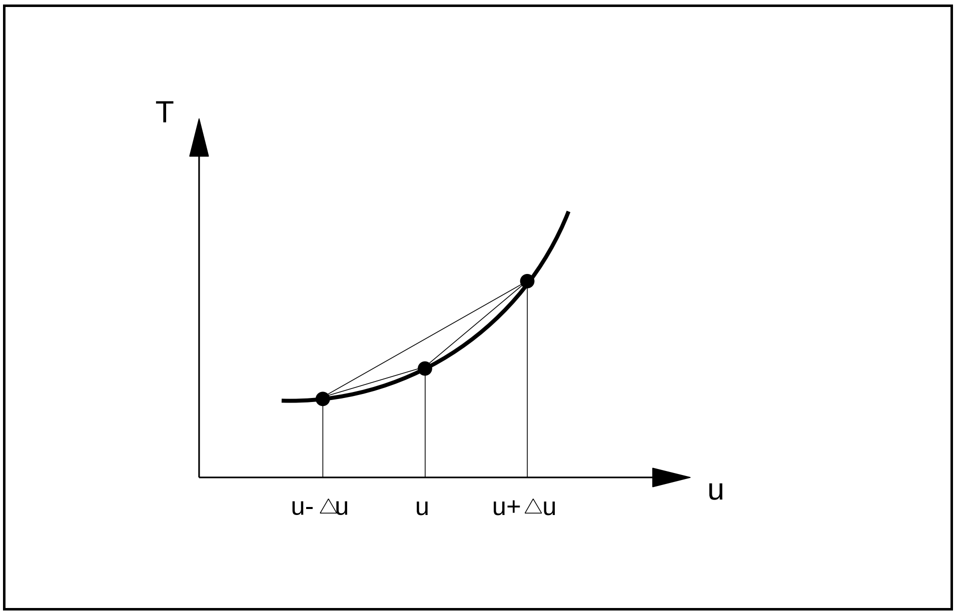

Figure 1

With the argument *u* replaced by time *t*, one of these approximations can be inserted as a difference approximation of the time derivative in the left hand side of the transient heat conduction equation (Equation 1).

Adding Equations 2 and 3 results in the following equation:

$$T(u+\Delta u)+T(u-\Delta u)=$$
$$2T(u)+\frac{2(\Delta u)^2}{2!}T''(u)+\frac{2(\Delta u)^4}{4!}T''''(u)+\ldots \tag{8}$$

An approximation of the second order derivative can be isolated from this Equation:

$$T''(u)=\frac{\partial^2 T}{\partial u^2}=\frac{\mathrm{T}\,(\mathrm{u}-\Delta\mathrm{u})\ -\ 2\,\mathrm{T}\,(\mathrm{u})\ +\ \mathrm{T}\,(\mathrm{u}+\Delta\mathrm{u})}{(\Delta\mathrm{u})^2}\ +\ \mathrm{O}\,[(\Delta\mathrm{u})^2] \tag{9}$$

With the argument *u* replaced by the space coordinate *x*, the right hand side of Equation 9, exclusive of its O-function, (written in bold) can be inserted as difference approximation of the second order space derivative in the right hand side of the transient heat conduction equation (Equation 1).

Using the forward approximation for the time derivative results in the following finite difference form of the transient heat conduction equation:

$$\frac{T(x,t+\Delta t) - T(x,t)}{\Delta t} = a\frac{T(x-\Delta x,t) - 2T(x,t) + T(x+\Delta x,t)}{(\Delta x)^2} \quad (10)$$

Errors

As a result of neglecting the higher order terms of the Taylor expansions above, the finite difference method will give solutions that deviate from the exact solution of the PDE. This difference is called the *discretization* or *truncation error*. The important thing is that the error decreases as Δu (i.e. Δt and Δx) tends to zero, that is the discretization error is some O[$(\Delta u)^n$]-function.

Another requirement of a good numerical method is that the discretization error does not increase from one iteration in time to another - that is the method should be *stable*. Stability depends on the discretization scheme and is discussed further in the lecture note on the so-called explicit and implicit numerical schemes.

Finally, one should keep in mind that computers are not able to give exact representations of the results of finite difference equations. Any result that has more digits that can be retained by the computer (i.e. most real numbers) is subject to a *round-off error*. Round-off errors will accumulate if the results of the calculations are generated on the basis of results from earlier time steps or iterations of the same calculations. While small space and time discretizations decrease the discretization errors, they also increase the total number of computations needed, and thus, may cause round-off errors to add up.